

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -45.2 °C

Global applicability domain: Inside

Local applicability domain index: 4.79e-01

Confidence level: 5.84e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Dichlorvos</div> <div>Measured: -60.0</div> <div>Predicted: -45.2</div>	<div>Image not found</div> <div>Tris(2-chloroethyl) phosphate</div> <div>Measured: -35.0</div> <div>Predicted: -30.9</div>	<div>Image not found</div> <div>Tris(2-chloroisopropyl)phosphate</div> <div>Measured: -40.0</div> <div>Predicted: -39.4</div>
<div>Image not found</div> <div>Naled</div> <div>Measured: 27.0</div> <div>Predicted: 18.1</div>	<div>Image not found</div> <div>Dimethylvinphos</div> <div>Measured: 69.5</div> <div>Predicted: 59.8</div>	